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14. ABSTRACT
This report summarizes the progress made in developing the theoretical underpinnings for a new theory of brittle fracture based upon an extension of continuum mechanics to the nano-scale. In contrast to classical fracture theories, the new theory predicts bounded crack tip stresses and strains by including a novel boundary condition arising from the jump momentum balance enforced on fracture surfaces which are modeled as dividing surfaces with excess physical properties including surface free energy, surface tension and surface entropy. As a result of the bounded crack tip stresses and strains, it was necessary to introduce a new notion of crack tip Energy Release Rate (ERR), a new fracture criterion based this new ERR and a method to estimate from first principles the corresponding Critical ERR (cERR). Estimates of the cERR for diamond, silicon and silicon-carbide compared favorably with published NIST data with no adjustable parameters.

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A central issue in the use of advanced materials in structural applications is their susceptibility to catastrophic failure due to fracture. Being able to predict when cracks will form, and when and how they will propagate is crucial to predicting material reliability in a service environment.

Classical linear elastic fracture mechanics (LEFM) has been utilized successfully for predicting crack initiation and quasi-static (slow) crack growth in many brittle structural materials. However, it has been shown to be inadequate when attempts are made to apply it in simplistic fashion under other situations such as to materials exhibiting significant ductility or viscoelasticity, or to cracks propagating dynamically (even in brittle materials), or to fatigue cracking. Moreover, as a physical theory, LEFM has a well known internal inconsistency. Namely, it is predicated upon the assumption of infinitesimal strains while simultaneously predicting singular strains and stresses at a fracture edge. Singular stresses are predicted even when the theory is generalized to the setting of finite elasticity. Additionally, LEFM predicts blunt crack tip opening profiles while experimental observation suggests crack tips should have sharp, cusp-shaped profiles.

Various strategies to circumvent this internal inconsistency of LEFM have been explored over the past fifty years, but few of them have explored the fundamental role that nanoscale, interfacial physics plays in understanding the mechanics of the region surrounding a crack edge. A central goal of the research effort has been to exploit in a variety of fracture scenarios a novel approach to modeling brittle fracture recently introduced by the Principal Investigators (PIs) that captures critical interfacial effects via their recently developed method for extending continuum mechanics to the nanoscale.

A primary objective of the proposed research was the formulation and combined analytical and numerical solution of a variety of canonical fracture and other interfacial boundary value problems. As that work progressed, it became evident that a new theoretical foundation for an energy based fracture criterion was required as well as a rigorous analysis of the fracture boundary value problem. This task consumed most of the effort of the final grant year and resulted in a new definition of the Energy Release Rate (ERR) and substantial progress towards developing an elegant new theory of its use as a fracture criterion along with a rigorous analysis of the corresponding analog within the new fracture theory of the canonical Griffith crack problem. What follows is a brief description of these developments.

The classical definition of the ERR was introduced in the setting of a static mode I (opening mode) crack in a linearly elastic body. It was subsequently generalized to treat quasi-statically growing cracks and then dynamically growing cracks in either linear elasticity (infinitesimal strains) or finite elasticity. In the latter case, the theory was always developed using a (stress free) reference configuration, and in all cases singular crack tip stresses and strains were assumed leading to a finite, non-zero flow of (mechanical) energy into the crack tip. Consideration was also given to cohesive zone models which remove stress and strain singularities and for which the ERR is replaced by the rate of working of the cohesive zone

stresses. However, for all of these theories, fracture surfaces were not modeled as dividing surfaces with excess physical properties.

The fracture theory being developed by the PIs endows the fracture surfaces with excess physical properties (momentum, internal energy, entropy, surface tension, etc) and incorporates a mutual body force correction to the differential momentum balance. These two modeling elements, the excess properties and the mutual force, together are intended to correct the bulk material constitutive behavior in a neighborhood of a fracture (dividing) surface for effects emanating from the long range intermolecular forces from the adjoining phases on either side of the fracture surface.

There have been a few previous attempts to develop fracture theories in which fracture surfaces are endowed with surface tension, internal energy, momentum and entropy, but none of them recognized the crucial role played by the jump momentum balance in deriving the “correct” fracture surface boundary conditions. In particular, these previous studies attempted to apply classical fracture surface boundary conditions along with the inclusion of fracture surface excess properties resulting in classical crack tip singular stresses and strains.

The new approach to modeling fracture studied under this AFOSR grant was introduced under the PIs previous AFOSR grant and described in the paper (1). That paper considered the classical static Griffith crack problem in the context of the new theory utilizing fracture surface excess properties and a mutual force correction to the differential momentum balance. The problem was formulated and studied within the deformed configuration under the assumption that the linear Hooke’s law could be used to model the bulk material properties away from the fracture region. It also used a fracture boundary condition dictated by enforcing the jump momentum balance across the fracture surfaces. Singular perturbation methods were used to derive from the jump momentum balance boundary condition a differential equation for the configuration of the (opened) fracture surfaces. All of the analyses and simulations presented in that paper were predicated upon the assumption that the model would predict bounded stresses and strains at the crack tip in contrast to classical fracture theories.

Subsequently, the PIs and their student T. Sendova began addressing the many theoretical questions left unanswered in (1). First they showed that the solutions derived via the singular perturbation methods and numerical simulations in (1) do in fact exhibit bounded crack tip stresses and strains giving a consistency result. Under the subsequent AFOSR project, the PIs addressed the question of showing a priori that the fracture boundary value problem resulting from the new theory must necessarily predict bounded crack tip stresses and strains and to determine which effect, the boundary condition derived from the jump momentum balance in the presence of crack surface excess properties or the mutual force correction to the differential momentum balance, is responsible for removing the crack tip stress and strain singularities seen in the classical fracture theories.

Against this backdrop, the principal accomplishments of this AFOSR project are summarized below.

(I) The PIs and T. Sendova proved various results associated with the canonical fracture boundary value problem considered in (1).

   a. They showed that the use of Hooke’s law in the deformed configuration was valid provided crack tip stresses and strains remain bounded and provided it is a valid approximation in a stress free reference configuration.

b. They then showed that the theory does indeed predict bounded crack tip stresses and strains when using the crack boundary condition following from the jump momentum balance under the assumption of crack surface excess properties (specifically, surface tension) and not adopting a mutual force correction to the differential momentum balance. This analysis involved several key ingredients: (i) pull the nonlinear fracture boundary value problem back to the reference configuration; (ii) linearize the differential and jump momentum balances in the reference configuration; (iii) employ integral transform techniques to derive an integrodifferential equation for the crack face displacement from the jump momentum balance; (iv) use generalized Fourier analysis to transform the boundary integrodifferential equation to an infinite linear algebraic system; (v) prove existence of solutions to this infinite linear system; (vi) prove that the solution of the infinite linear system leads to bounded crack tip stresses and strains. They also slowed that just using the mutual force correction and the classical (traction free) fracture boundary condition does not, in general, lead to bounded crack tip stresses and strains. It is still an open question (though, undoubtedly true) as to whether using both the jump momentum balance boundary condition and the mutual force correction leads to bounded crack tip stresses and strains. The PIs and Sendova are working to fill in this gap in the theory. An interesting feature of this analysis is that is demonstrates that certain aspects of the new fracture theory are more easily addressed in the deformed configuration while others in the reference configuration. This work will appear in (3).

(II) One glaring omission in (1) was consideration of an appropriate fracture criterion within the new fracture theory. Two possible routes to a fracture criterion were explored under this ending AFOSR contract.

a. Given the above proof that the new theory predicts bounded crack tip stresses and strains, a tantalizing new approach to deriving a fracture criterion could be based upon the crack tip stress. Specifically, it would postulate that crack growth can occur only when the predicted crack tip stress reaching the critical cleavage (bond) strength of the (brittle) material. The crack tip stress could be estimated either from an asymptotic theory as developed in (1) or from direct numerical solution of the nonlinear fracture boundary value problem. It remains to test such a fracture criterion against experimental data.

b. Classical fracture mechanics is based upon use the Critical Energy Release Rate (cERR) as a fracture criterion. However, that notion was derived in the context of singular crack tip stresses and strains leading to a non-zero mechanical power flux into the crack tip. It became evident that a new notion of energy release rate was needed for the new theory. Development of that theory was initiated under this project and continued into the new start. A candidate for the cERR was postulated (for brittle crystalline materials), being the rate of working needed to break chemical bonds (short range intermolecular forces) plus the rate of working required to overcome the long range intermolecular forces (per unit crack advance).

(III) A key step in the implementation of an ERR fracture criterion is the ability to determine the cERR. A method for calculating the cERR for brittle materials was developed in (2) and tested against published (NIST) data for diamond, silicon and silicon carbide. Excellent agreement was achieved with no adjustable parameters, that is, all necessary model parameters (specifically the required Hamaker constants and surface tensions for the three materials considered) were obtained from the literature. This work will appear in (2).

THESES AND DISSERTATIONS

The Ph.D. student support under this AFSOR project, Ms. Tsvetanka Sendova, is writing her Ph.D. dissertation based upon the theoretical developments described above. She is scheduled to defend her dissertation in June 2008 and graduate in August 2008. Based upon the results she obtained on this project, she has been offered (and has accepted) a postdoctoral position at the Institute for Applied Mathematics and Its Applications at the University of Minnesota beginning in September 2008.

REFERENCES

(1) E.-S. Oh, J. R. Walton & J. C. Slattery, A Theory of Fracture Based upon an Extension of Continuum Mechanics to the Nanoscale, *J. Appl. Mech.,* **73** (5), pp. 792-798, 2006.

(2) K.-B. Fu, E.-S. Oh, T. Sendova, J. C. Slattery, J. R. Walton, The Critical Energy Release Rate Based upon an Extension of Continuum Mechanics to the Nanoscale, submitted to *Int. J. Frac.*.

(3) K.-B. Fu, T. Sendova, J. C. Slattery, J. R. Walton, Analysis of a Theory of Fracture Based upon an Extension of Continuum Mechanics to the Nanoscale, in preparation.